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Improving the scaling and performance of GROMACS on HECToR using single-sided communications.

Document Title: Final Report

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Date: 05/12/2013
Version: 1.0

Abstract

GROMACS (GROningen MAchine for Chemical Simulations) is a molecular dynamics package primarily designed for simulations of proteins, lipids and nucleic acids. It was originally developed in the Biophysical Chemistry department of University of Groningen, and is now maintained by contributors in universities and research centres across the world. GROMACS is one of the fastest and most popular software packages available, and can run on CPUs as well as GPUs. It is free, open source released under the GNU General Public License.

GROMACS has been parallelised using a hybrid MPI + OpenMP model, which is able to scale to several thousand nodes. There are at least three different parallelisation methods used in the code that can be selected at runtime. This project worked to improve the performance of the different parallelisation methods used on the HECToR system by implementing some internal communication routines with single-sided equivalents, using the SHMEM communication library. Results show that the replacement of MPI routines by one-sided equivalents does not affect performance, although current limitations in the programming model and the implementation limits performance benefit.

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1 Introduction

This report documents the work performed during the dCSE project titled "**Improving the scaling and performance of GROMACS on HECToR using single-sided communications**". The project has been undertaken at EPCC, The University of Edinburgh, in conjunction with Professor Berk Hess, from the KTH Royal Institute of Technology, Stockholm, and Dr Andrew Turner and Dr Ruyman Reyes from EPCC, University of Edinburgh.

The project attempted to reduce the computational resources required to undertake scientific simulations, enabling more efficient use of the resources provided by the HECToR service (and other HPC systems), and reducing the runtime required to undertake simulations for large scale problems.

1.1 GROMACS

GROMACS[1] is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.

It is primarily designed for biochemical molecules like proteins, lipids and nucleic acids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the non-bonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers.

GROMACS supports all the usual algorithms a user would expect from a modern molecular dynamics implementation.

It also features high performance compared to all other programs. Since in GROMACS 4.6, the innermost loops are written in C using intrinsic functions that the compiler transforms to SIMD machine instructions, to utilize the available instruction-level parallelism. These kernels are available in both single and double precision, and are supported by all the different kinds of SIMD support found in x86-family processors available in January 2013.

GROMACS also supports CUDA-based GPU acceleration using NVIDIA devices. The parallel implementation uses MPI and OpenMP to scale up to thousands of cores.

1.2 HECToR

HECToR[2] (HECToR), a Cray XE6 computer, is the UK National Supercomputing Service. This project utilised the Phase 3 incarnation of the system. Phase 3 of HECToR consists of 2816 nodes, each containing two 16-core 2.3 GHz 'Interlagos' AMD Opteron processors per node, giving a total of 32 cores per node, with 1 GB of memory per core. This configuration provides a machine with 90,112 cores in total, 90TB of main memory, and a peak performance of over 800 TFlop/s.

1.3 Test Cases

Two different test cases have been used for benchmarking the GROMACS simulation package.

1.3.1 NADP-DEPENDENT ALCOHOL DEHYDROGENASE in water

The first test case used in this study is solvated alcohol dehydrogenase (ADH) in a cubic unit cell (134,000 atoms in total). This system has issues with load balancing.

1.3.2 Grappa test case

The second test case used in this study is a water/ethanol mixture (Grappa). This test case is available in three sizes and shows good load balancing, as the system is very homogeneous.

1.3.3 Regression tests

In addition to the performance benchmarks mentioned, we have made extensive use of the GROMACS test suite, with various combinations of threads and ranks, to ensure correctness of the code at every stage.

1.4 Objective

We aim to improve the performance of the inter-task communications of GROMACS by replacing the calls to standard MPI two-sided communication routines with a single-sided communication interface which can be implemented using different single-sided communication libraries (for example, SHMEM, Fujitsu Tofu interconnect, Infiniband verbs). On HECToR we will implement the interface using calls to the single-sided, Cray SHMEM communication routines. SHMEM has been selected as it is currently available in a form that can give excellent performance on Cray MPP machines (such as HECToR) and is also currently an area of active development through the OpenSHMEM[3] initiative. OpenSHMEM currently have a number of reference implementations but no high-performance versions of their libraries.

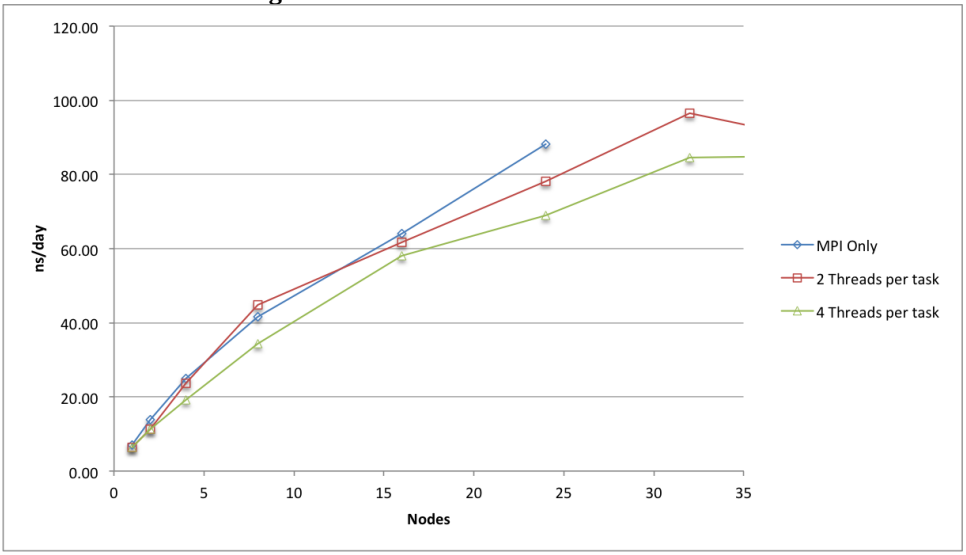
For the remainder of this report we will first provide an initial performance analysis and benchmarking of GROMACS and SHMEM in Section 2. We will provide implementation details in Section 3, with a description of each one of the implemented changes. Then, in Section 4 we analyse the performance of the implementation, showing profiling results and final benchmarking results for the provided test cases.
To conclude, conclusions and final remarks are provided in Section 5.

2 Initial Performance

3.1 Initial GROMACS Benchmarking

Our initial benchmarking is based on the ADH Cubic test case supplied by the GROMACS developers using both pure MPI and hybrid MPI+OpenMP (with multiple OpenMP threads per MPI task). The performance as a function of number of HECToR nodes is shown in Figure 1.

Figure 1: Performance of GROMACS on HECToR Phase 3 for ADH Cubic test case using automatic PME load balancing.



The data shows that the pure MPI version of GROMACS scales well up to 24 nodes (768 tasks) for this benchmark. The hybrid version with two OpenMP threads per MPI task generally shows lower absolute performance but is able to exploit more cores (up to 32 nodes, 1024 tasks). Using higher numbers of MPI tasks for this benchmark is problematic due to issues matching the parallel domain decomposition to the larger task count.

3.2 Initial GROMACS Profiling

The current GROMACS code has been profiled using CrayPAT[4] while running the ADH Cubic benchmark for a variety of core counts. We have used tracing experiments to profile the code and gather MPI message statistics.

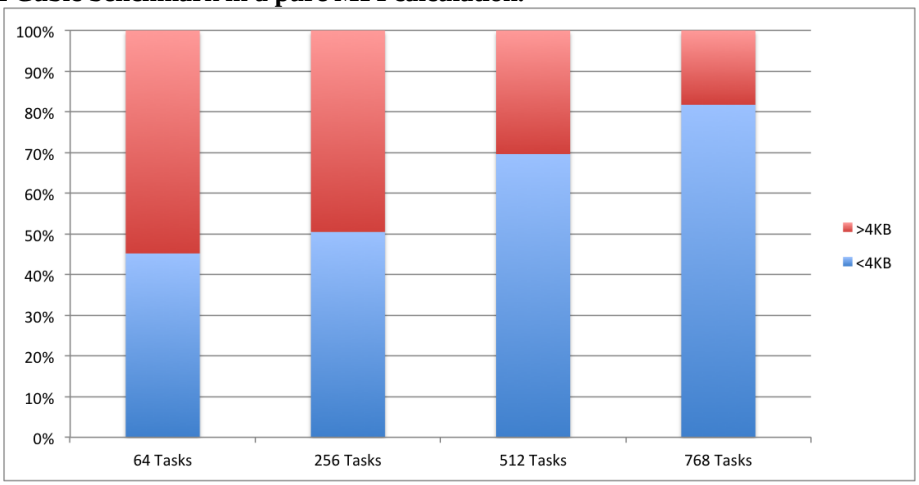
Table 1 provides an overview of where time in the code is spent when using both 64 and 512 MPI tasks. We can see that, as expected, when we increase the number of tasks, the MPI communications become a significant portion of the calculation. In particular, the MPI point-to-point routines (MPI_Sendrecv and MPI_Recv) take up the majority of the communication time.

Table 1: Sampling results for GROMACS 4.6.0 on HECToR Phase 3 running the ADH Cubic test case. % values indicate average amount of time spent in named routine.

Function	64 MPI Tasks	512 MPI Tasks
USER	76.7%	49.1%
Main	76.7%	49.1%
MPI	22.5%	47.4%
MPI_Recv	4.6%	27.1%
MPI_Sendrecv	6.7%	11.3%
MPI_Alltoall	1.2%	5.0%
MPI_Waitall	9.6%	2.9%
MPI SYNC	0.8%	3.5%
MPI_Alltoall	-	1.5%
MPI_Bcast	-	1.5%
SYSTEM ROUTINES	0.0%	0.0%

Figure 2 shows how the message size distribution changes for the MPI_Sendrecv routine as a function of number of MPI tasks. At 512 MPI tasks 70% of the messages are small (<4KB) and at 768 tasks this share has increased to over 80%.

Figure 2: Distribution of MPI_Sendrecv message sizes as a function of number of MPI tasks for the ADH Cubic benchmark in a pure MPI calculation.



3 SHMEM Implementation

This work focused on improving the performance of the inter-process communication using SHMEM. The implementation details are described in the following subsections. The majority of the effort invested in the implementation has been devoted to circumvent the considerations listed below without breaking the overall GROMACS modularity.

3.1 SHMEM considerations

To integrate the SHMEM implementation with the ongoing GROMACS development, we forked the 4.6.3 release of the package repository and created a new public development branch with the integrated SHMEM improvements.

A build-time option has been added to the GROMACS CMake which enables the experimental SHMEM support (GMX_SHMEM). This option tests for the existence of either Cray or OpenSHMEM support in the platform, and enables the appropriate macro definitions if it is found. Although the performance figures shown in this report are based on the Cray SHMEM implementation, the code can be built in platforms using the OpenSHMEM implementation.

3.1.1 Programming model limitations

The logically shared, distributed memory access (SHMEM) routines provide low-latency, high-bandwidth communication for massively parallel programs. Applications implemented in SHMEM follow the Single Program Multiple Data (SPMD) model, hence, no process can be added or removed from the group, and all processes execute the same application.

This contrasts with the GROMACS approach of using MPMD to solve the Particle-Mesh-Ewald method (PME) on a predetermined subset of nodes. To facilitate the work, we have disabled this feature in the command line and we assume that all nodes perform the PME (*-npme 0*).

This may hinder performance at larger node counts, limiting the scaling to the performance of the AlltoAll routine.
Although it would be possible to modify GROMACS so that all nodes compute PP but only a subset of them will compute the PME, the development effort required would exceed the time allocated for this project. Some ideas on how to modify the GROMACS source to allow the usage of PP and a subset of PME are provided in the Appendix A.

3.1.2 Memory allocation

Another consideration for using SHMEM is the requirement of using symmetric memory for all the inter-process communication routines. Symmetric memory is allocated using special routines (*shmalloc*, *shrealloc* and *shfree*). This requires identifying all the possible allocations of the variables involved in communications and replacing them with their symmetric counterparts.
In addition, the symmetric memory routines contain an implicit global barrier, thus we had to ensure that these allocations were performed simultaneously (and with the same size) across all ranks.

Figure 3 Memory layout of a SHMEM program. Notice that the Symmetric Heap (SHMEM in the figure) has the same starting base address in all ranks. When a symmetric allocation routine is called in all PEs, the heap grows symmetrically. Since the pointer to buff is the same, put/get routines can put data using the same address in all ranks.

To allocate symmetric memory within GROMACS, we have added symmetric variants of the already existing routines (*snew*, *srenew*, *smalloc*, *srealloc*, *sfree*). The equivalents of these routines have an extra *sh_* before the name (*sh_snew*, *sh_srenew*,

sh_smalloc, *sh_sfree*). Note that allocation routines do not check if the allocated size across all ranks is the same.

The macro *shrenew* has been created for convenience, and uses the *shmem_get_max_alloc* routine to compute the maximum amount of memory requested across all ranks. The *shmem_get_max_alloc* routine swaps two synchronization arrays (one for odd, other for even calls) to allow consecutive calls to the maximum routine without extra synchronization costs.

```
void * sh_renew_buf(gmx_domdec_shmem_buf_t * shmem, void * buf, int *
alloc, const int new_size, const int elem_size)
{
      void * p;
      int global_max;
      global_max = shmem_get_max_alloc(shmem, new_size);
      if (global_max > (*alloc))
      {
            (*alloc) = over_alloc_shmem(global_max);
            sh_srenew(buf, (*alloc) * elem_size);
      }
      p = buf;
      return p;
}
```

3.1.3 Using put or get

SHMEM offers support for both Put and Get one-sided operations. Put is typically much faster than Get, and we have made our best effort to use Put as much as possible. However, it is important to note that Put and Get require different arguments on the symmetric heap. Put requires the pointer to where the data have to be written to be in the symmetric heap, whereas Get is the pointer to where the data has to be read the one that have to reside in the symmetric heap.
In some parts of the SHMEM implementation, we have opted to use Get over Put to reduce the number of symmetric memory allocations and facilitate synchronization. A good example of this is the implementation of the PME part of the code.
The Get version of relevant Send Receive routines can be selected using the GMX_SHMEM_USE_GET macro.

3.1.4 Supporting tools available

Cray environment provides several tools for performance analysis, which include support for SHMEM.
However, debugging SHMEM codes is not an easy task. Despite having access to the Cray comparative debugger, sometimes tracking dangling pointers has been an exhausting task. Porting a code to SHMEM, in particular one as large as GROMACS, moving incrementally memory allocations to the symmetric heap is not an easy task, and prone to errors. When a symmetric memory pointer is de-allocated with a non-symmetric routine, there is no immediate error in the free: The symmetric heap just become inconsistent and may (or may not) produce errors in future allocations. This complicates debugging, as errors may appear far from the point where the real problem is.
We have made extensive use of the GROMACS regression tests with various configurations to ensure the application returns correct results.

3.2 SHMEM Control structure

A data structure holding all the control information required to the SHMEM communications has been created. It is detailed below.

```
typedef struct {
      /* These buffers are used as temporary
           interchange space for SHMEM routines */
    int  * int_buf;
    int    int_alloc;
    real * real_buf;
    int    real_alloc;
    real * rvec_buf;
    int    rvec_alloc;
    void * byte_buf;
    int    byte_alloc;
    /* An event array to synchronize shmem operations */
    shmem_flag_t * post_events;
    shmem_flag_t * done_events;
    /* Array of locks (i-th is the lock for the i-th pe) */
    shmem_flag_t * lock;
    /* wkr and sync arrays for max_alloc routine */
    long * max_alloc_pSync1, * max_alloc_pSync2;
    int  * max_alloc_pWrk1,  * max_alloc_pWrk2;
} gmx_domdec_shmem_buf_t;
```

This structure is initialised the *init_shmem* routine, and can be freed with the *done_shmem* routine, following the example of other data structures inside the code.
The intermediate buffers are not used in the final implementation, although we keep them in the data structure to facilitate possible future work.
The *max_alloc_{pSync1, pSync2, pWkr1, pWrk2}* arrays are used to synchronize the *shmem_int_max_to_all* routine used to synchronize the buffer size for the reallocation.
The data structure is created when the simulation starts, and it is associated with the communication data structure. It is later associated with specific DD, PD or PME control data structures to facilitate access to intermediate pointers.

3.3 Replacement of SendRecv operations in the Domain Decomposition part of the code

The first task undergone in this work was to implement the Send Receive operations used in the Domain Decomposition part of the code with SHMEM equivalents.
The DD part uses pulsed communication, which makes the code a bit simpler and reduces the number of communication calls.
The Domain Decomposition data structure was extended with a pointer to a SHMEM control data structure, which contains pointers to synchronization arrays, temporary buffers, locks, and other control structures used through the program. The structure is initialised when creating the domain decomposition structure.
The routine *dd_sendrecv_{int,real,rvec}* were modified so that they use SHMEM routines instead of MPI when the build-time option is enabled.
Although integer interchange routines are implemented in SHMEM they do not represent a major advantage on the performance and they are disabled by default. This first approach used a temporary symmetric buffer per-data type, to avoid replacing all the allocations of the code, as shown in the following listing:

```
void shmem_void_sendrecv(gmx_domdec_shmem_buf_t* shmem,
                         void* buf_s, int n_s, int rank_s,
                         void* buf_r, int n_r, int rank_r)
{
      shrenew(shmem, shmem->{type}_buf, &(shmem->byte_alloc), n_s);
      shmem_lock(shmem, rank_s);
      if (n_s) {
            shmem_{type}_put(shmem->{type}_buf, buf_s, n_s, rank_s);
      }
      shmem_set_post(shmem, rank_s);
      shmem_wait_post(shmem, _my_pe());
      if (n_r) {
            memcpy(buf_r, shmem->{type}_buf, n_r * sizeof(real));
      }
      shmem_set_done(shmem, rank_r);
      shmem_clear_post(shmem, _my_pe());
      shmem_wait_done(shmem, _my_pe());
      shmem_clear_done(shmem, _my_pe());
      shmem_unlock(shmem, rank_s);
}
```

To ensure there is enough space to store the communication buffer we call our own *shrenew* routine, which computes the maximum allocation required across all ranks and reallocates memory if required.
The sender PE acquires the lock to gain access to the buffer and put the data on the destination PE. The receiver PE will wait (*shmem_wait_post*) until the sender sets a particular flag (*shmem_set_post*). Then, the data in the symmetric buffer is copied to the reception buffer. Both PE can now set an additional flag to ensure reception (*set_done*, *wait_done*), and, finally, unlock the buffer.
Using the initial global barrier ensures synchronization.
The Figure below depicts the communication pattern for this implementation when interchanging data in the forward direction.

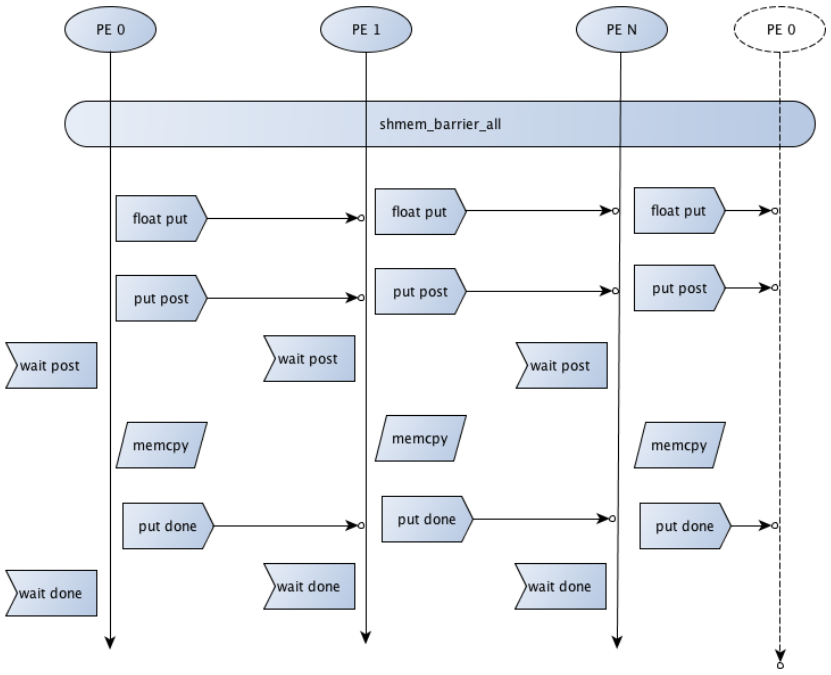


Figure 4 Communication diagram of a forward pulse. After all PE reach the global barrier, each PE puts data on the forward node, and then waits to receive data from the backward node.

This approach poses several performance problems. The obvious one is the requirement of a global barrier to ensure synchronization. This forces each PE to wait for the rest, hindering performance on unbalanced systems such as the ADH test case.
Also, the requirement for the receiver to copy data from the symmetric buffer to the real destination buffer introduces additional overhead, proportional to the amount of data transmitted.
Due to these restrictions, we moved to Send/Recv routines without intermediate buffers, therefore modifying the original GROMACS code to use symmetric allocation routines (see Section 3.3.1).

3.3.1 Memory allocations

Our first step to improve the performance of this approach was to move the memory allocations of those buffers used in the DD communication to the symmetric heap.
This required, among others, the creation of new *init_state* and *done_state* routines implemented the aforementioned symmetric allocation.
The coordinates and velocities (x and v vectors) of the state have been ported to symmetric memory, as they are communicated within *dd_move_f* and *dd_move_x* routines[1].
Most of the data structures used in communications are allocated as follows:

```
 if (local_buffer_size < number_of_elements * size)
{
    local_buffer_size = number_of_elements * size;
    buffer = realloc(buffer, local_buffer_size);
}
```

Since the number of elements across all ranks is not constant, the size of the local buffer in the MPI version is reallocated only on those ranks requiring it. This is not possible on the SHMEM, as it will produce (a) deadlocks if not all processors need to reallocate and (b) incorrect symmetric addresses if the size is not the same in all ranks.
To avoid these problems, we re-implement the reallocation computing the global maximum of the buffer required and reallocating the same amount in all ranks.

```
int max = shmem_get_max_alloc(dd->shmem, local_buffer_size);
shrealloc(buffer, max);
```

Note that the reallocation routine contains a global barrier.
To avoid the constant reallocation of buffers in the domain decomposition, we try to move buffer reallocations outside loops when possible, and work with temporary buffers in the heap if not.
For those buffers whose size depends either on the total number of charges or the total number of atoms, we pre-compute the maximum number of charges and atoms per rank and reuse this value whenever possible, reducing the total calls to the maximum collective.

[1] However, the random part of the X update and the P vector for CG minimization still reside on the heap, reducing the symmetric memory footprint.

The DD control data structure has been extended with a variable that keeps track of the maximum number of atoms in a node. This variable is updated when *nat_home* changes, and its value reused in many places to reduce the calls to the *max_to_all* collective.

3.3.2 Offset swap

Some of the Send Receive operations used within the domain decomposition involved sending data from a buffer and receiving there on a different one. This can be a problem when using one-sided communications. Let's take the following simple MPI example. First, we communicate the size of the buffer. Then we do the same with the buffer, according from the data received before.
Note that the position in the receiver changes depending on the received information, and that the sender does not now where the data is going to be written in the receiver.

```
for (int i = 0; i < nelems; i++)
{
  MPI_SendRecv(to_send, 1, MPI_INT, destination[i], 0,
               to_recv, 1, MPI_INT, source[i], 0,
               MPI_COMM_WORLD, &stat);
  MPI_SendRecv(buf[i], to_send, MPI_INT, destination[i], 0,
               rec[pos], to_recv, MPI_INT, source[i], 0,
               MPI_COMM_WORLD, &stat);
  pos += to_recv;
 }
```

If we port these Send Receive operations by simply writing the information from the sender to the receiver (using a put operation with no intermediate buffer) we will end up with incorrect results, as the position where the sender is writing does not necessarily match the position the receiver is expecting.
To overcome this problem, the Sender needs to know where the offset in the receiver to put the data. In our implementation, the receiver puts the offset on the sender, and then waits for the data to be sent.
However, it is required to change the signature of the *dd_sendrecv_{rvec,real,int}* functions, so that the offset to the symmetric buffer can be differentiated from the pointer address itself. New *dd_sendrecv_{rvec,real,int}_off* have been created for that purpose. The code shown below illustrates the interchange of sizes and offset that happens before sending the data.

```
if ( recv_size > 0 )
{
      /* Receiver: Put offset on sender */
      shmem_int_p(&rem_off, off_r, recv_nodeid);
      /* Receiver: Put size on sender */
      shmem_int_p(&rem_size, recv_bufsize, recv_nodeid);
      /* Receiver: Ensure delivery (but not reception!) */
      shmem_fence();
}
if ( send_size > 0 )
{
      /* Sender: Wait for offset from receiver */
      shmem_int_wait(&rem_size, -1);
}
```

Another implementation problem related with the offset interchange is that sometimes the base pointer where the routine has to put to or get the data from is not symmetric across all ranks. For example, in some situations, some ranks will receive the data in place while others need to receive the data on a temporary buffer.
This problem notably appears in some routines used in the domain decomposition.
Depending if the implementation uses put or get, which buffer we are writing to needs to be communicated. The appropriate code can be enabled with pre-processor directives (USE_GETMEM or USE_PUTMEM macros).
The implementation for the interchange of the *x* buffer in the *dd_move_x* routine is outlined below:

```
static int rparams[2] = { -1,-1 };
static int call = 0;
int tmp[2];
shmem_wait_for_previous_call(dd->shmem, &call, dd->neighbor[d][0]);
tmp[0] = cd->bInPlace;
tmp[1] = nat_tot;
// First stage: Communicate in place and offset
dd_sendrecv_int_nobuf(dd, d, dddirForward, tmp, 2, rparams, 2);
{
      rvec * rem_rbuf = rparams[0]?x:comm->vbuf2.v;
// Second stage: Communicate the data
      dd_sendrecv_rvec_off(dd, d, dddirBackward,
                           buf, 0, ind->nsend[nzone+1],
                           rem_rbuf,
                           rparams[0]?rparams[1]:0,
                           ind->nrecv[nzone+1]);
}
call++;
```

After ensuring that both receiver and sender are on the same iteration, we communicate the value of the *inPlace* variable and the offset to the Forward direction, so that the senders have the positions where they have to write data in the next Send Receive operation. Notice that the sender will use either *x* or the temporary buffer to put the data depending on the value received from the receiver in the previous stage.

3.3.3 Synchronization

Our next step was to eliminate the global barrier before the each call to the Send Receive operation.
Since in the domain decomposition all PEs call the Send Receive operations at the same point in the code – but not at the same point in time – we can replace the global barrier with a call counter. Whenever a rank calls a Send Recv operation, it checks the sender and destination values for this routine counter, and waits until the value match its own. When the Send Recv operation finishes, it increases the counter.
This mechanism enables two ranks to synchronize without affecting the rest, thus reducing the overhead on poorly balanced codes. We have implemented this mechanism as a subroutine (*shmem_wait_for_previous_call*) and use it thorough the SHMEM parts of the code as a replacement for barriers whenever possible.

```
void shmem_wait_for_previous_call (gmx_domdec_shmem_buf_t * shmem,
                                   int * call, int rank)
{
   while ( (shmem_int_g(call, rank)) != (*call) )
   {
            sched_yield();
   }
}
```

Using *sched_yield* forces the current process to go back to the end of the pending queue. This may help the Cray MPI progress thread to continue process messages, or other threads to access to the CPU while waiting – which is particularly interesting for OpenSHMEM implementations.

3.3.4 Final Send/Receive implementation

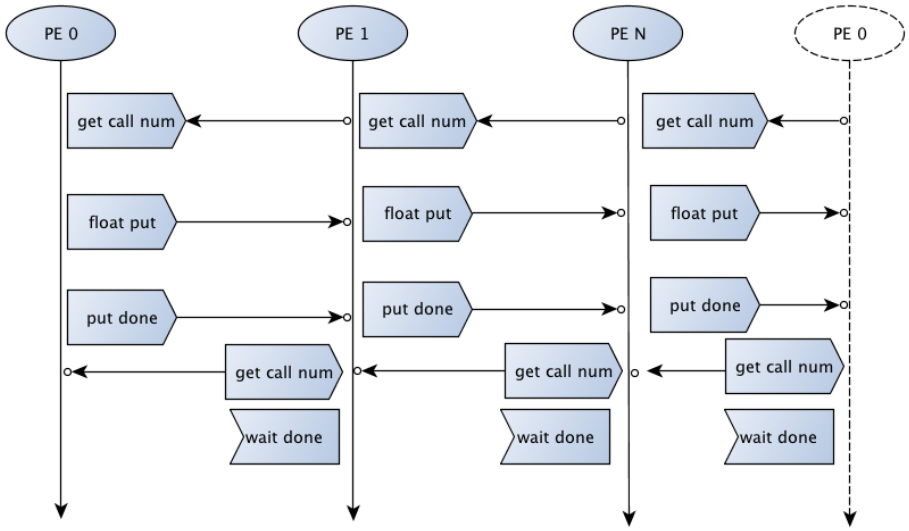


Figure 5 Call diagram of the optimized Send Receive operation implemented in SHMEM.

For illustrative purposes, Figure above illustrates the call diagram of the Send Receive operation using N ranks, where the i-th rank sends data to the i+1%N rank, and receives from the i-1%N rank. Where possible, the sending/receiver part of the routine is only executed if there is data to send/receive.

3.3.5 Send Receive in two directions simultaneously

In some situations inside the DD part, it is necessary to send information in both forward and backward direction. If performed simultaneously, it provides an important performance benefit. The *dd_sendrecv2_rvec* routine implements this operation in MPI making use of non-blocking Send / Receive operations.

We have implemented similar functionality in the new SHMEM implementation using non-blocking SHMEM put operations to transfer the information, producing a specific *dd_sendrecv2_rvec_off* routine that puts data in both directions simultaneously.

3.3.6 Reducing the impact of memory re-allocation

To reduce the impact of the implicit barrier during the memory re-allocation, we took advantage of the fact that the size of the communication buffers grows during the

initial steps of the simulation, but later it stabilises around a number. This enabled us to implement a simple heuristic that detects the number of times the size of a particular buffer has been changed. If in a certain number of iterations this size has not changed, we disable the reallocation (and the call to the global max collective).
In case that at some point after disabling the re-allocation, the size of the buffer is increased over the last time it was re-allocated, the code stops the simulation with a descriptive message.
Developers can modify the value of the MAX_SAME macro to set the number of times the reallocation is called with the same size before disabling it. The listing below shows an example of the implementation of this simple heuristic when reallocating the sate data structures.

```
{
static int nsame_natoms = 0;
if (nsame_natoms < MAX_SAME)
{
 int max =  shmem_get_max_alloc(dd->shmem, state_local->natoms);
 if (max > state_local->nalloc)
 {
    dd_realloc_state_shmem(state_local, f, max);
    nsame_natoms = 0;
}
 else
 {
    nsame_natoms++;
 }
}
else
{
  if (state_local->natoms > state_local->nalloc)
  {
   gmx_fatal(FARGS, " New natoms value greater
                      than old_natoms, increase MAX_SAME \n");
  }
 }
}
```

3.4 Replacement of SendRecv operations in the Particle Decomposition part of the code

The particle decomposition (PD) part of the code is relatively simpler than the DD part, with less number of lines and a simpler communication pattern. However, since this part of the code may be deprecated in the near future, we have only focused on correctness and not performance.

3.4.1 Replacement of memory allocations

In addition to those memory allocations already moved for the DD part of the code the PD part of the code makes use of temporary buffers for some communications. These buffers have been moved now to the symmetric heap. Some refactoring work was required to move the buffer allocations to ensure all ranks execute the allocation instructions.
For example, in the *setup_parallel_vsites* routine, there are several calls to the *add_to_vsite_list* routine, which in turns reallocates either the *left_import_construct*

or the *right_import_construct*. These reallocations will deadlock if not performed symmetrically.
The SHMEM implementation creates the symmetric buffers after the aforementioned loop and copies the initial data to this symmetric buffer.
In addition, send and receive buffers - which in the MPI implementation were allocated to the local size in each rank – are allocated to the maximum size of the buffer across all ranks.
Since the PD part of the code only uses the *state_global* variable, instead of than replicating the global state on local states as the DD part of the code does, the allocation of this global state buffer had to be moved to the symmetric heap as well.
However, the *state_global* structure is used to load data from the input files, a task performed only by the master node. This implies that the symmetric memory cannot be allocated at this point.
Although the logically sound point to do this reallocation would be the *set_state_entries* routine, which fixes the state data structure after the file has been initialised and it is called by all ranks, this breaks the modularity of the code, due to the fact that all variants of the code (DD, PD, non-pararallel) go through this routine.
In order to keep the modularity we have modified the *partdec_init_local_state* routine, which initialises the state when using PD, so that the existing coordinates and velocities are moved to the symmetric heap at this point, copying the data from the global to the local state, rather than reassigning de pointers as the MPI version does. Since this is in the initialisation phase, we do not expect to cause major performance problems.

```
int i;
int max_atoms =
        shmem_get_max_alloc(cr->pd->shmem, state_global->natoms);
sh_snew(state_local->x, max_atoms);
sh_snew(state_local->v, max_atoms);
cr->pd->max_atoms = max_atoms;
if (state_global->natoms)
{
  if (state_global->x)
  {
    for (i = 0; i < state_global->natoms; i++)
      {
        copy_rvec(state_global->x[i], state_local->x[i]);
      }
      sfree(state_global->x);
      state_global->x = state_local->x;
  }
 …
```

3.4.2 Replacement of the Send Receive routines

Majority of the Send Receive operations use the *gmx_tx_rx* routine. We have created a set of type-specific versions of these routines and implemented them using our previously developed Send Receive routines.
Those situations where offset were involved have been solved using the same mechanism as in the DD part (*_off* variants of the routines).
To optimise the MPI implementation, some movement routines implemented a deferred send and wait using non-blocking communication, as shown below, in an attempt to send and receive from both directions at the same time.

```
start = cgindex[cur];
nr    = cgindex[cur+1] - start;
gmx_tx(cr, GMX_LEFT, cg_cm[start], nr*sizeof(cg_cm[0]));
start = cgindex[next];
nr    = cgindex[next+1] - start;
gmx_rx(cr, GMX_RIGHT, cg_cm[start], nr*sizeof(cg_cm[0]));
gmx_tx_wait(cr, GMX_LEFT);
gmx_rx_wait(cr, GMX_RIGHT);
```

This is not required in the SHMEM implementation, as there is no need for a receive statement. The SHMEM implementation only calls the offset version of the *gmx_tx_rx* routine, as shown below

```
int start_s = cgindex[cur];
int nr_s = cgindex[cur+1] - start_s;
int start_r = cgindex[next];
int nr_r = cgindex[next+1] - start_r;
gmx_tx_rx_real_off(cr, GMX_LEFT, *cg_cm, start_s * DIM, nr_s * DIM,
                   GMX_RIGHT, *cg_cm, start_r * DIM, nr_r * DIM);
```

It is worth noting, from the above code snippet, that pointer arithmetic should be taken into account when using offset routines. The offset of the memory is based on the size of the datatype. In the snippet, since the communication routine is of type real and the *cg_cm* vector is of type *rvec* (which is, in turn, a *real[NDIM]* vector), the offset have to be adjusted accordingly. This happens also in the *move_rvecs* routine, where the original code simply used *vecs[index[cur]]* but the code using offset interchange requires a not-so-readable offset of *index[cur] * DIM*.

```
gmx_tx_rx_real_off(cr, GMX_RIGHT, *(vecs),
                   index[cur ] * DIM, HOMENRI(index, cur )*DIM,
                   GMX_LEFT, *(buf), index[prev] * DIM,
                   HOMENRI(index, prev)*DIM);
```

3.5 Replacement of Send/Receive operations in the Particle Mesh Ewald part of the code

The final part of this project was focused on the implementation of the PME part of the code using the SHMEM routines. Due to time constraints, we focused only on those routines strictly appearing on the profiling results containing Send/Receive operations.

3.5.1 MPI communicators

All communications used in the PME part of the code use a separate communicator, with routines using this indexing rather than the global one.
Since there are no subgroup capabilities on SHMEM, we had to convert the communicator IDs to global IDs, usable by SHMEM routines.
The *pme_get_global_id* routine implements that conversion using the *MPI_Group_translate_ranks* routine, as shown below.

```
    int pme_get_global_id(pme_atomcomm_t *atc, int nodeid)
    {
      int global, ret;
      int group, wgroup;
```

```
      ret = MPI_Comm_group(atc->mpi_comm, &group);
      if (ret != MPI_SUCCESS)
      … error check …
      ret = MPI_Comm_group(MPI_COMM_WORLD, &wgroup);
      … error check …
      ret = MPI_Group_translate_ranks(group, 1, &nodeid,
                                          wgroup, &global);
      … error check …
      return global;
    }
```

The routine first gets a pointer to both the PME group and the world group, and then translates the nodeid rank number to the global rank number.
We have experienced some difficulties with these MPI routines, producing random crashes when called many times, thus, we try to minimise its use as much as possible.

3.5.2 Send/Receive operations

Send/Receive operations in the PME part of the code are encapsulated on calls to the *pme_dd_sendrecv* routine. The destination and source nodes for each of these calls are determined by the shift of the communication, using the *node_dest* and *node_src arrays*. These values are converted to global ranks with the *pme_get_global_id* routine.
We have reused the SHMEM Send/Receive routines from previous sections to implement the PME communications.
However, in this case Send/Receive operations are not necessarily called by all ranks at the same point in the code, since some ranks may not communicate at a particular shift. Since the *shmem_wait_for_previous_call* is useless in this situation, other mechanism has been used.
In addition, Send/Receive operations in the MPI implementation rely on separate tags for each shift to differentiate messages, which is not possible in the SHMEM implementation.

3.5.3 Redistribution of coordinates and charges

The redistribution of coordinates and charges in the PME part is performed by the *dd_pme_redist_x_q* routine. This routine put the charges and forces on to a buffer and then sends/receive them across all nodes involved in the PME, as shown below.

```
// Reallocate buffers
…
// Communicate the count
…
for (i = 0; i < nnodes_comm; i++)
{
 int scount = atc->count[commnode[i]];
 pme_dd_sendrecv(atc, FALSE, i,
                      &scount, sizeof(int),
                      &atc->rcount[i], sizeof(int));
 atc->n += atc->rcount[i];
}
```

```
// Copy data to send buffer
…
buf_pos = 0;
// Communicate charges and coordinates
for (i = 0; i < nnodes_comm; i++)
```

```
{
 scount = atc->count[commnode[i]];
 rcount = atc->rcount[i];
 if (scount > 0 || rcount > 0)
 {
   if (bX)
   {
        /* Communicate the coordinates */
        pme_dd_sendrecv(atc, FALSE, i,
                            &pme->bufv[buf_pos],
scount*sizeof(rvec),
                            &atc->x[local_pos],
rcount*sizeof(rvec));
   }
   /* Communicate the charges */
   pme_dd_sendrecv(atc, FALSE, i,
                        pme->bufr           +           buf_pos,
scount*sizeof(real),
                        atc->q            +            local_pos,
rcount*sizeof(real));
   buf_pos   += scount;
   local_pos += atc->rcount[i];
 }
}
```

Since not all nodes had to communicate in all shifts, and not all nodes have the same destination and source in all shifts, it is possible that a node that does not communicate in the first shift, has to do it on the second shift. Since there are no tags in the SHMEM implementation, this processor may write on the buffer while a node from the previous shift is still reading data, potentially causing corruption or even deadlocks if the offset or done flags are incorrectly modified.

To avoid this problem, instead of using the traditional Send/Receive replacement, we decided to follow a slightly different approach this time, and modify the redistribution routine itself rather than the low-level one.

The SHMEM implementation is depicted below. The main idea is that, since we are using one-sided communications, we do not need to communicate the buffer sizes, we only need to put the data in the proper place.

In this case we had two options: Either the sender ranks putting data on the appropriate position of the receiver or the receiver getting data from the correct positions in the sender.

Since using get in this case required only the PME buffers to be allocated in the symmetric memory we opted in this case to implement the routine using get instead of put.

Instead of using Send/Receive to get the value of *rcount*, we moved the *count* array to the symmetric heap so the receiver can get it directly from the sender.

The values of count are computed in the routine *pme_calc_pidx_wrapper*. We added a *recount_call* field to the *atc* structure, so we can ensure that we are getting data from the correct iteration. We also added an *acum_rcount* field to the *atc* structure, which is initialised with the accumulated values of the count value (i. e $a[i] = a[i-1] + count[i], \forall i > 0$).

In this alternative implementation of the redistribution, where the active role is in the receiver side, the sender needs to wait until the receivers had retrieved the data. The more we can defer this wait, the better we can hide the cost of the PME

communication. Currently we have implemented this wait at the end of the redistribution routine, but a detailed study of the code may reveal other approaches.
The wait is implemented using a counter. The static variable *used* is initialised with the total count of data that will be retrieved from the node.
Each receiver uses an atomic operation to decrease this value in the sender.
The sender will wait until the value of used is zero again before invalidating the buffer. The ready flag tells acts as a barrier, ensuring that the *receiver* can read the used variable, and the data from the count is array is valid.
This approach allows the receiver to get the data from the sender completely independent from the sender, once the ready flag is set.

```
// Reallocate buffers
…
/* Get the num of elements to receive by this PE */
for (i = 0; i < nnodes_comm; i++)
{
      int src  = pme_get_global_id(atc,atc->node_src[i]);
      int rcount;
      shmem_wait_for_previous_call(atc->shmem, atc->recount_call,
                                   src);
      rcount = shmem_int_g(&atc->count[atc->nodeid], src);
      atc->rcount[i] = rcount;
      atc->n += rcount;
}
// Copy data to send buffer
...
buf_pos = 0;
// Communicate charges and coordinates
for (i = 0; i < nnodes_comm; i++)
{
  int src  = pme_get_global_id(atc,atc->node_src[i]);
  while ( shmem_int_g(atc->recount_call, src)
              != *(atc->recount_call) )
  {
    sched_yield();
  }
  used += atc->count[commnode[i]];
}
shmem_int_p(&ready, 1, _my_pe());
shmem_quiet();
for (i = 0; i < nnodes_comm; i++)
{
 int scount = pme_get_global_id(atc, atc->count[commnode[i]]);
 int rcount = pme_get_global_id(atc, atc->rcount[i]);
 if (rcount > 0)
 {
   {
    shmem_fence();
    while (!shmem_int_g(&ready, src))
    {
      sched_yield();
    }
   }
   int rem_buf_pos = shmem_int_g(&atc->acum_count[i], src);
   if (bX)
   {
     shmem_getmem(&atc->x[local_pos][0],
                  &pme->bufv[rem_buf_pos][0],
```

```
                    rcount * sizeof(rvec), src);
    }
    shmem_float_get(&atc->q[local_pos],
                     &pme->bufr[rem_buf_pos], rcount, src);
    local_pos += atc->rcount[i];
    shmem_int_add(&used, (-1) * rcount, src);
   }
   {
       shmem_fence();
      // Wait until all processes have retrieved the data
       while ( (volatile) used )
       {
             sched_yield();
       }
     // Invalidate the buffer data
     shmem_int_p(&ready, 0, _my_pe());
     shmem_quiet();
}
```

To reduce the amount of time spent waiting for other ranks to finish, we slightly modified the part where the *rcount* is computed, so that several ranks could be checked simultaneously, instead of waiting for a particular one to finish, which allow us to hide the imbalance in the PME part of the code.

```
int remaining[nnodes_comm];
int src[nnodes_comm];
int rem_count = nnodes_comm;
int i = 0;
for (i = 0; i < nnodes_comm; i++)
{
      remaining[i] = 1;
      src[i] = pme_get_global_id(atc,atc->node_src[i]);
}
do
{
 for (i = 0; i < nnodes_comm; i++ )
 {
 if (remaining[i] == 1)
  {
   /* Get the num of elements to receive by this PE */
   int rcount;
   if(shmem_int_g(atc->recount_call, src[i])== *(atc->recount_call) )
   {
    remaining[i] = 0;
    rem_count--;
    rcount = shmem_int_g(&atc->count[atc->nodeid], src[i]);
    atc->rcount[i] = rcount;
    atc->n += rcount;
   }
  }
 }
} while (rem_count > 0);
```

4 Performance analysis of the implementation

4.1 Profiling

We have made profuse use of the Cray profiler while working on the implementation in order to focus our development effort in those areas where its effect would be beneficial. Some partial analysis and outputs are shown below to illustrate the evolution of the development process.

4.1.1 Initial implementation

Our initial implementation of the Send/Recv routines in the Domain Decomposition part of the code revealed the unfeasibility of using buffers locals for the Send Receive operations, due to the excessive overhead of the buffer reallocation and the global barrier.

Group	% Time	Imb. Time %	Name
USER	87.8%		
SHMEM	6.1%		
	4.5%	56.5%	shmem_int_max_all
	1.2%	8.08%	shmem_barrier_all
	0.3%	2.0%	shmem_put
MPI	5.8%		
	5.0%	47.5%	MPI_Sendrecv

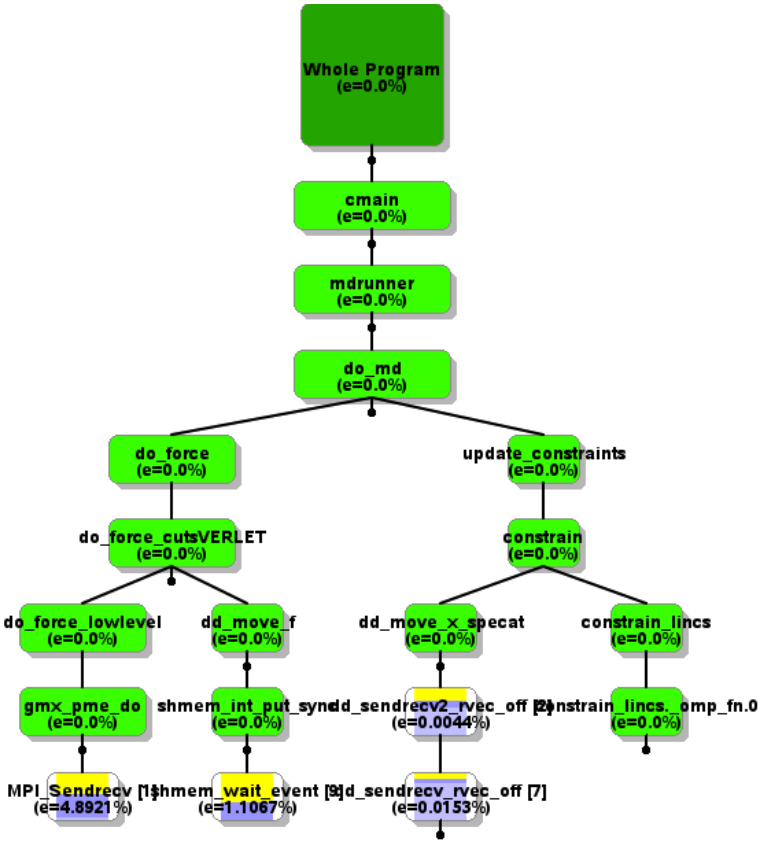
The profiler results above, using 8 cores of a HECToR node with only 10000 iterations of the ADH test code, revealed the limitations of this approach. Notice that, despite only porting part of the domain decomposition send receive routines, the barrier and maximum are already 5.7% of the total 6.1% of the time spent in SHMEM routines. Also, we are only using intra-node communications, where we expect a similar behaviour between SHMEM and MPI.

4.1.2 Improved Send Recv in domain decomposition

After replacing the buffered Send Recv routines by non-buffered ones, and reducing the number of calls to the maximum collective, the profiler output looked as follows (obtained with the same conditions than the previous case)

Group	% Time	Imb. Time %	Name
USER	88.1%		
SHMEM	5.9%		
	3.1%	64.0%	shmem_wait_event
	1.4%	58.2%	shmem_int_wait
	0.7%	81.3%	shmem_int_wait_until
	0.4%	48.9%	shmem_int_max_to_all
MPI	5.8%		
	5.0%	47.5%	MPI_Sendrecv

Notice that the maximum collective has nearly disappeared, and the SHMEM time is spent in the *wait_event* routine. The *calltree* (shown below) reveals that most of the time was spent in the two-way send receive operations, which at this point were implemented using first a pulse forward and then a pulse backwards. We expect that when using more than one node, the maximum collective would be again the bottleneck due to its increased cost.



4.1.3 Final profiling analysis

Group	1 node, 32 cores		16 node, 512 cores	
	MPI (s)	SHMEM (s)	MPI (s)	SHMEM (s)
Total	2231.71	2189	480.01	530.52
USER:	1775.49 (79.6%)	1979 (90.4%)	144.00 (30.0%)	195.54 (37%)
MPI	411.31 (18.4%)	31.90 (1.5%)	257.38 (53.6%)	54.46 (10.3%)
MPI_SendRecv	310.99 (13.9%)	31.76 (35.5%)	109.46 (22.8%)	49.83 (9.4%)
MPI_AlltoAll	43.90 (2.0%)		126.25 (26.3%)	
MPI_Sync	44.90 (2.0%)	1.83 (0.1%)	78.62 (16.4%)	1.68 (0.3%)
SHMEM		61.53 (2.8%)		65.69 (12.4%)
shmem_wait		27.87 (1.3%)		11.16 (2.1%)
shmem_int_g		11.82 (0.5%)		22.71 (4.3%)
Total comm.	411.31 (18.4%)	93.43 (4.2%)	336 (70%)	121.83 (23%)

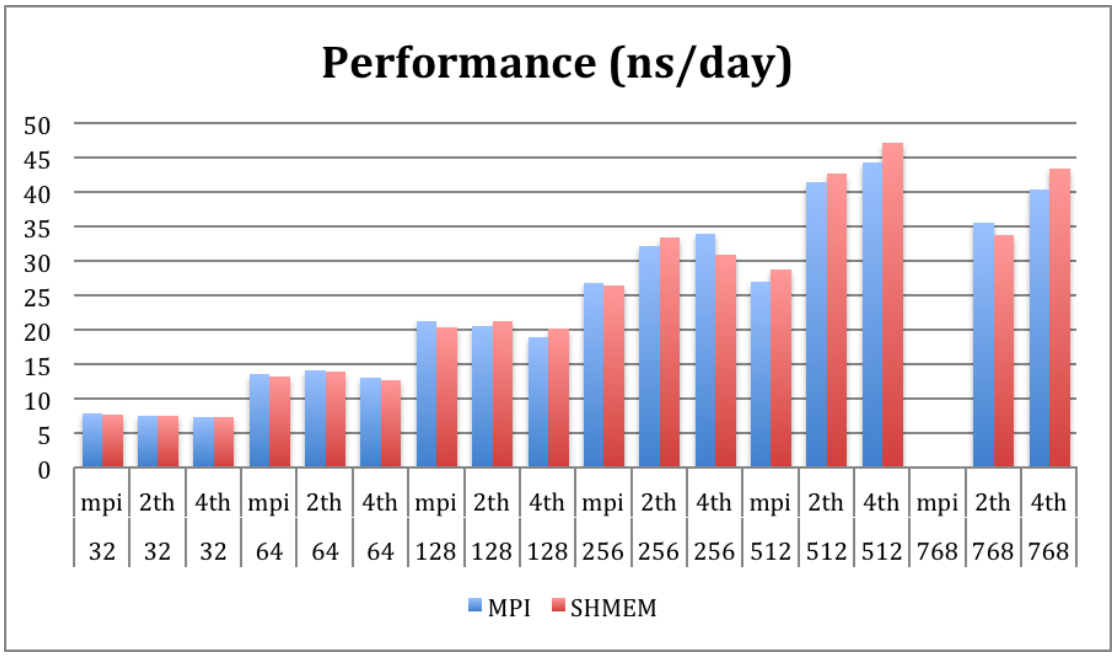
The table above shows the time spent in the different groups of profiling analysis according to Craypat when using 1 and 16 nodes with 100000 iterations of the ADH test case. The last row of the table, Total comm, shows the sum of the time spent in MPI and the time spent in SHMEM. Notice the drastic reduction in the time spent in communication when using SHMEM. However, it is worth noting that the USER time has increased. This is because of the active waiting of the *shmem_wait_for_previous_iteration*. This time comes from the imbalance of the application and the problem being executed. The imbalance time in the MPI

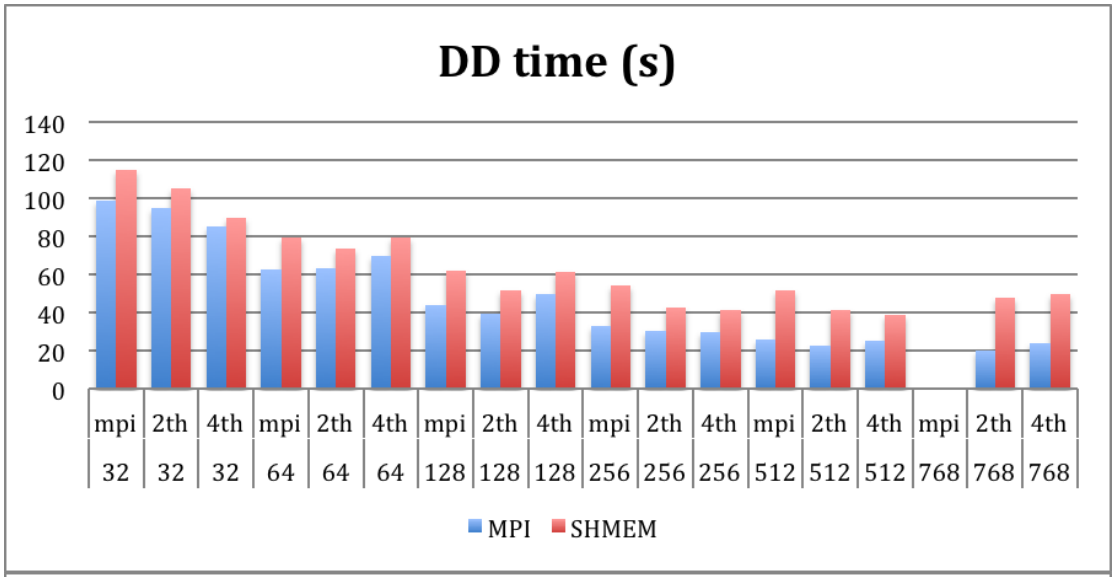
implementation is shown as time spent in *SendRecv* or Recv, but this comes to user code in our implementation. Notice however that the shmem_wait routines, which also are affected by imbalance, are included on the SHMEM time.
It is worth noting also that the maximum collective does not show up in the profiling report. The heuristics added to reduce the number of overall synchronisation improve the performance of the SHMEM implementation. Disabling these heuristics increases the walltime of the SHMEM implementation up to a 20%.
This experimental data make us believe that the fine-tuning of these heuristics may improve the performance. In particular, tuning these heuristics for the particular conditions of each execution (maybe by the means of a user variable or configuration) could enhance the performance of the different executions.

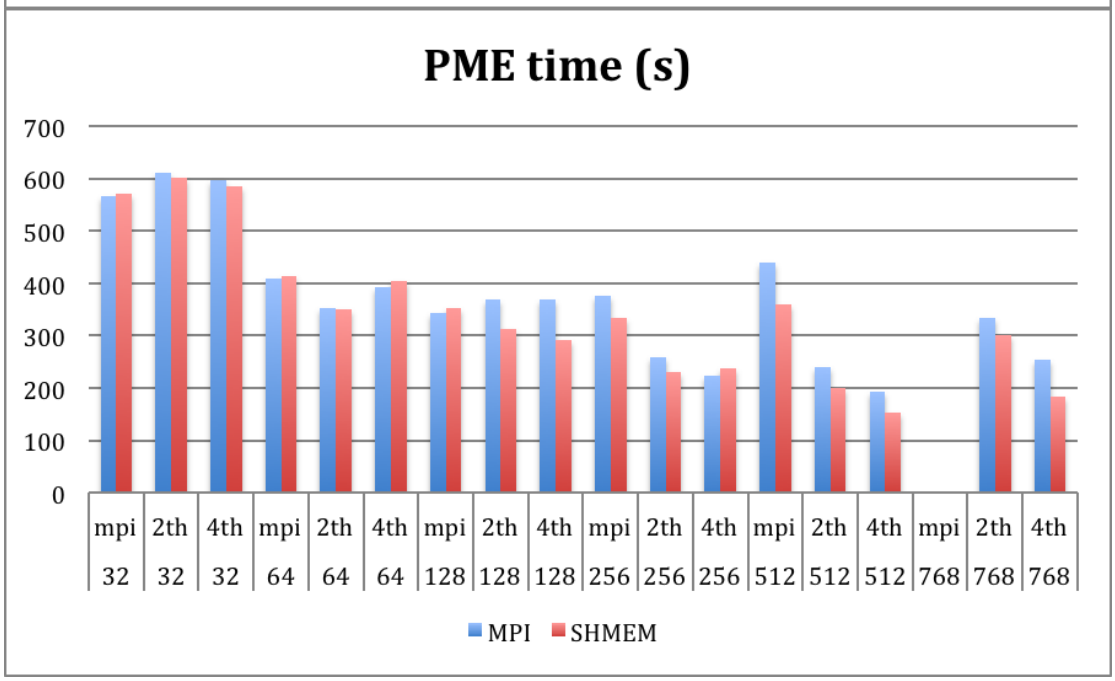
4.2 Performance Benchmarks

The following subsections illustrate the performance obtained with the benchmark codes. This performance figures are extracted from the timing table provided by GROMACS. Performance (ns/day) is the overall performance of the execution, DD is the time spent in Domain Decomposition and PME is the time spent computing the PME.
Since we are using these internal counters, the imbalance of the application will affect time measurement, thus, even the lower time spent in communication will be hidden by its effects.

4.2.1 ADH test case

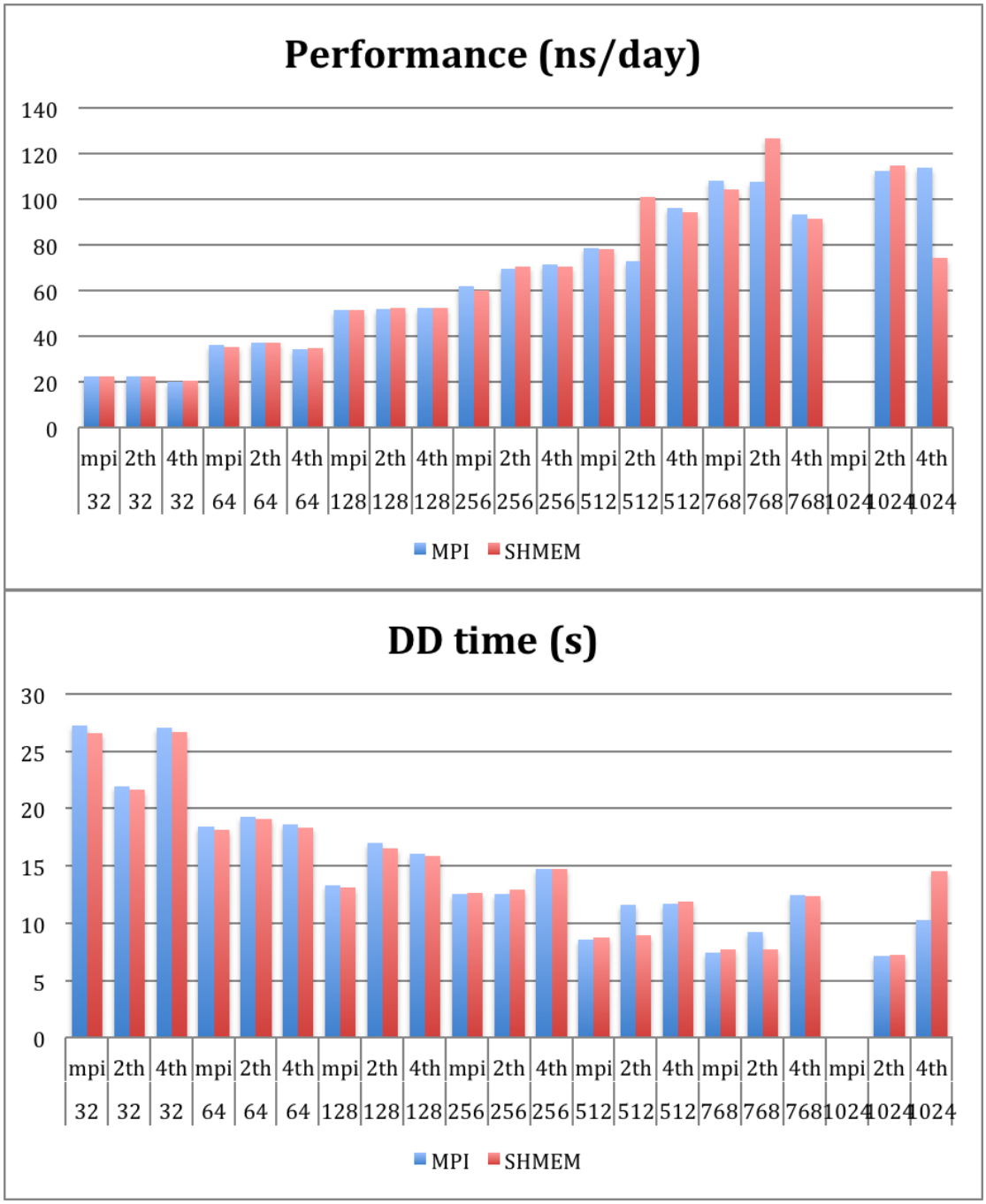


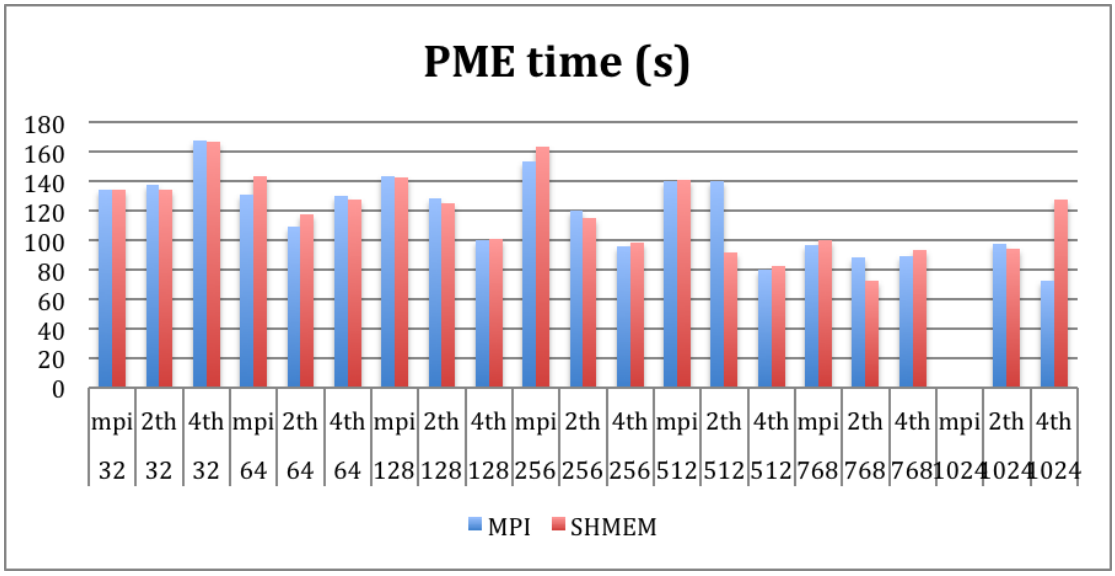




4.2.2 Grappa test case

45k molecules


Performance (ns/day)
140
120
100
80
60
40
20
0
mpi 32
2th 32
4th 32
mpi 64
2th 64
4th 64
mpi 128
2th 128
4th 128
mpi 256
2th 256
4th 256
mpi 512
2th 512
4th 512
mpi 768
2th 768
4th 768
mpi 1024
2th 1024
4th 1024
MPI
SHMEM
DD time (s)
30
25
20
15
10
5
0
mpi 32
2th 32
4th 32
mpi 64
2th 64
4th 64
mpi 128
2th 128
4th 128
mpi 256
2th 256
4th 256
mpi 512
2th 512
4th 512
mpi 768
2th 768
4th 768
mpi 1024
2th 1024
4th 1024
MPI
SHMEM



5 Summary

In this project we have explored the different possibilities of implementing a one-sided programming model in a large code base, such as GROMACS. Although initially the idea sounded promising, various implementation details affected the final performance results.

We have presented a paper, titled "Introducing SHMEM into the GROMACS molecular dynamics application: experience and results", in the PGAS 2013 conference (held in Edinburgh) where we present the results and the recommendations for other PGAS developers.

Many decisions in the existing code, aimed to improve the performance of the MPI implementation, limited the applicability of SHMEM.

For example, some routines compressed data into a buffer in order to produce a single MPI Send Receive call.

This is not required in SHMEM, where it would be possible to directly send the data to other ranks in separated put calls with lower overhead.

Ideally, in SHMEM programs the memory is allocated at the very beginning of the program, thus the implicit barriers are not a problem. However this is not possible in GROMACS, where the data that is communicated is reallocated during the execution.

In addition, the SPMD model of SHMEM contrasts with the MPMD approach of GROMACS. Although it would be possible to replicate the allocations of the PME nodes into non-PME nodes and vice versa, the development cost would excess the time allocated for the project.

An alternative implementation using MPI one-sided communications, recently adopted in the MPI 3.0 standard, may be seen as better suited given the circumstances. The development effort and analysis performed during this project will leverage the implementation costs a future MPI one-sided approach, as the major areas of improvement and the refactoring has been already performed.

6 Acknowledgements

This work was supported by Dr Berk Hess at KTH.

This project was funded under the HECToR Distributed Computational Science and Engineering (CSE) Service operated by NAG Ltd. HECToR – A Research Councils UK High End Computing Service - is the UK's national supercomputing service, managed by EPSRC on behalf of the participating Research Councils. Its mission is to support capability science and engineering in UK academia. The HECToR supercomputers are managed by UoE HPCx Ltd and the CSE Support Service is provided by NAG Ltd.

References

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[2] HECToR website, http://www.hector.ac.uk/
[3] OpenSHMEM website, http://openshmem.org/
[4] Cray Profiling and Analysis Tools documentation in HECToR, http://www.hector.ac.uk/support/documentation/userguide/tools.php#craypat

Appendix A: PME-only nodes implemented in SHMEM

Discussions with the development team have raised some ideas to overcome the limitation of using the same number of PME and PP nodes in the SHMEM implementation. Some of these ideas are described below as future reference

6.1 Using MPMD execution

Building separate PP and PME binaries and using the aprun MPMD capabilities to launch two separate executables on the same MPI_COMM_WORLD communicator may overcome the limitations of the memory allocation. Changes in GROMACS would be simple.
However, current Cray SHMEM implementation does not support multiple binaries, thus, this is not viable on HECToR.

6.2 SHMEM subgroups

Discussions on the OpenSHMEM mailing lists are being held on adding support for subgroups of processors in SHMEM. Whether this will include in future releases or not is yet to be officially communicated.
If the SHMEM standard adopts this functionality, the GROMACS SHMEM implementation could be easily modified to support this feature.

6.3 PME in a subset of nodes but PP on all nodes

Since the PME part of the code only requires an intermediate communication buffer allocated in symmetric memory, and it is currently allocated at the beginning of the program, it would be possible to use the PME part only on a subset of the nodes. However, it is not possible to not execute the PP part, as it contains many memory reallocations that cannot be easily replicated on the PME-only nodes.
The current implementation decides before starting the molecular dynamics simulation if a particular node is a PP or PME only. If the number of PME-only nodes is set to zero, the current implementation forces that all nodes are PP and PME.
A detailed analysis of the code reveals that it would be possible to modify the code enabling a new alternative where PP nodes can be PP-only or PP and PME.
Rather than using a Split Communicator operation when splitting the ranks in the domain decomposition, the PP communicator would continue to be the whole rank, and the PME rank would be the subset. The communication between PME and PP nodes would need to be adjusted to ensure the proper redistribution of data. Currently, The PP nodes check whether if they are PME also and, if not, they communicate the forces to the PME nodes. This check, both in sender (*dd_partition_system*) and receiver (*dd_forces_lowlevel*), would need to be modified to acknowledge the possibility of PP+PME nodes or PP-only nodes.
However, the most complex part of this modification is adding the code required to perform the PME in a subset of nodes without using the PP part of the code.
Since the current PME-only or PP-PME decision is held before the PP part, it would be necessary completely refactor the PP part to (1) disable the current PME implementation which does not communicate the forces but assumes local memory and (2) create a call to the PME-only part of the code after the force computation and before the receive of the forces from the PME-only nodes.

These changes require a noticeable effort and a deep collaboration with the GROMACS team, as it affects the development of future versions of the software. Since the GROMACS package is currently suffering a major re-factoring, this feature would need to be discussed in the future.